

Krein-Space Formulation of \mathcal{PT} -Symmetry, \mathcal{CPT} -Inner Products, and Pseudo-Hermiticity

Ali Mostafazadeh

Department of Mathematics, Koç University,
34450 Sariyer, Istanbul, Turkey
amostafazadeh@ku.edu.tr

Abstract

Emphasizing the physical constraints on the formulation of a quantum theory based on the standard measurement axiom and the Schrödinger equation, we comment on some conceptual issues arising in the formulation of \mathcal{PT} -symmetric quantum mechanics. In particular, we elaborate on the requirements of the boundedness of the metric operator and the diagonalizability of the Hamiltonian. We also provide an accessible account of a Krein-space derivation of the \mathcal{CPT} -inner product that was widely known to mathematicians since 1950's. We show how this derivation is linked with the pseudo-Hermitian formulation of \mathcal{PT} -symmetric quantum mechanics.

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1 Introduction

“In theoretical physics, there are a number of ideas that are periodically (re)discovered and then forgotten.” This was pointed out to me by George Sudarshan when I was a graduate student. By now, I have encountered a few concrete examples of these rediscoveries. I have also realized that sometimes they undergo mutations while they are repeated/reproduced and follow an evolutionary pattern in time. Occasionally they lead to an improved version of a previously known but forgotten idea that has a wider domain of application. Such

rediscoveries are by no means inferior to genuine discoveries, for they may be useful in dealing with certain problems that their previous versions could not handle.

I have elaborated on a recent example of such a “rediscovery” in [1]. It has to do with a recent version of the old notion of “a pseudo-Hermitian operator” used in the context of indefinite-metric quantum theories [2] – [4] and indefinite-metric linear spaces [5, 6, 7], namely the one proposed in [8, 9]. The main purpose for introducing this notion was to understand the spectral properties of a class of \mathcal{PT} -symmetric Hamiltonians [10]. The ensuing developments have not only achieved this purpose and led to a consistent formulation of unitary quantum systems based on a general class of non-Hermitian¹ Hamiltonians [12, 13, 14, 15], but perhaps more importantly played a central role in obtaining a complete solution of one of the oldest problems of modern theoretical physics, namely the problem of devising a genuine quantum mechanical treatment of Klein-Gordon and similar fields [11].

The key ingredient of the new notion of a pseudo-Hermitian operator is that it does not rely on a fixed pseudo-metric. Indeed the treatment of these operators given in [8, 9] involves constructing all possible compatible pseudo-metric operators that are associated with a pseudo-Hermitian operator H . In particular, whenever possible it yields the form of the associated positive-definite metric operators and the corresponding inner products that render H self-adjoint [9, 17].

In [16], the authors propose an alternative construction for a positive-definite inner product for a class of \mathcal{PT} -symmetric Hamiltonians. Although the point of departure and the approach leading to the inner product of [16], i.e., the so-called \mathcal{CPT} -inner product, are different from those of [9], as shown in [18, 13] this inner product belongs to a special class of those constructed in [9]. See also [17].²

The purpose of this paper is two fold: Firstly, I wish to draw attention to the physical constraints that need be imposed on any mathematical framework that aims at describing a unitary \mathcal{PT} -symmetric or pseudo-Hermitian quantum system. Secondly, I wish to show, using a minimal amount of mathematical formalism, that indeed the discovery of the \mathcal{CPT} -inner product [16] is another example of the “rediscoveries” I eluded to above. As far as I could trace, its original form appeared in a series of papers [19] by Rolf Nevanlinna published between 1952 and 1956. Nevanlinna’s construction is reviewed in mathematics [6, 7] as well as physics [3, 4] literature. It was indeed discussed by Japaridze [20] in 2001 in the context of \mathcal{PT} -symmetry, rediscovered by Bender, Brody, and Jones [16] in 2002, employed by Albeverio and Kuzhel [21] in 2004, and more recently by Tanaka [22, 23] in

¹We will follow the terminology used in the subject, and call a linear operator “Hermitian” if it is represented by a Hermitian matrix in a standard basis of the vector space it acts in. Below, we will give a precise definition.

²A concrete demonstration of the fact that there are physically acceptable inner products that do not belong to the set of \mathcal{CPT} -inner products is given in [15].

2006.

In what follows, I will first outline the physical constraints that limit the vast and virtually unbounded arena of mathematical possibilities for the problem and then give an accessible derivation of Nevanlinna's positive-definite inner product. This will in turn provide an opportunity to discuss various aspects of the problem, e.g., the connection to the pseudo-Hermitian formulation, the justification for the diagonalizability of the Hamiltonian, and the issue of the boundedness of the (pseudo-)metric operator.

2 Must Quantum Observables Be Hermitian?

In 1918, when Einstein received Weyl's letter asking his opinion on the latter's paper on gauge theories, Einstein's response was the following [24]: "Except for the agreement with reality, it is in any case a grand intellectual achievement." Einstein's reaction to Kaluza's 5-dimensional unification of gravity and electrodynamics was not different [25]. These are two instructive examples of how demanding physical considerations can become when mathematics is used to attack a particular physical problem. The same is true about quantum mechanics. It is not a lucky accident that out of the infinity of possibilities for function spaces that mathematicians are so eager to use in dealing with various problems in applied mathematics, it is only the (separable) Hilbert space that was found suitable by von Neumann to formulate quantum mechanics [26]. This was dictated by the physical constraints. Today, the same highly restrictive physical constraints persist in formulating a quantum theory based on a non-Hermitian Hamiltonian. Therefore, it seems necessary to seek for appropriate mathematical models only from among those that are compatible with the physical constraints.

A central objective of the recent study of \mathcal{PT} -symmetric Hamiltonians is to devise a quantum theory in which the dynamics is generated by the usual time-dependent Schrödinger equation,

$$i\hbar\frac{\partial}{\partial t}\Psi(z,t) = H\Psi(z,t), \quad t \in \mathbb{R}, \quad z \in \mathbb{C}, \quad (1)$$

where the Hamiltonian operator H is a Schrödinger operator,

$$H = -\frac{d^2}{dz^2} + v(z), \quad (2)$$

with a complex-valued potential $v : \mathbb{C} \rightarrow \mathbb{C}$, such as [10]

$$v(z) = -(iz)^N, \quad N \in \mathbb{R}^+. \quad (3)$$

The state vectors Ψ of the theory belong to a function space \mathcal{V}_Γ that, as we explain below, is defined using a certain contour Γ in complex plane \mathbb{C} . Specifically, Γ is obtained from

the real axis \mathbb{R} by an invertible deformation. As is common practice, we shall often identify Γ and a parameterized (piecewise regular) curve $\gamma : \mathbb{R} \rightarrow \mathbb{C}$ such that $\Gamma = \{\gamma(x) | x \in \mathbb{R}\}$. The most convenient γ is the one corresponding to the arc-length parametrization of Γ . We will assume that $\lim_{x \rightarrow \pm\infty} \gamma(x) = \infty$, where the second ∞ stands for the point at infinity, and that Γ is symmetric about imaginary axis whenever v is \mathcal{PT} -invariant, i.e., $v(r)^* = v(-r)$ for $r \in \mathbb{R}$, [13].

The function space \mathcal{V}_Γ has the following properties.

- (1) It is a complex vector space;
- (2) It includes the domain of H at least for all potentials v for which the eigenvalue problem

$$H\Psi_n(z) = E_n\Psi_n(z), \quad z \in \Gamma, \quad (4)$$

viewed as a holomorphic differential equation and solved along Γ is well-posed [27]. The latter condition is fulfilled provided that one imposes a set of appropriate boundary conditions at the infinities $\gamma(\pm\infty)$ of Γ . For typical polynomial potentials considered in the literature [28, 29], one requires a sufficiently rapid, typically exponential, decay at the infinities:

$$|x| \rightarrow \infty \quad \text{implies} \quad |\Psi(\gamma(x))| \rightarrow 0 \text{ exponentially}; \quad (5)$$

- (3) It is endowed with an appropriate complete metric such that the domain of H for all potentials with the properties mentioned in (2) is dense in \mathcal{V}_Γ . This is usually achieved by selecting a norm, i.e., promoting \mathcal{V}_Γ to a Banach space. In particular, given the boundary condition (5), one can view the state vectors Ψ as elements of the separable Hilbert space $L^2(\Gamma)$, i.e., the space of square-integrable functions $\Psi : \Gamma \rightarrow \mathbb{C}$, [30, 13], where Γ is viewed as a one-dimensional submanifold of $\mathbb{C} = \mathbb{R}^2$ with the metric (and hence integral measure) induced from the Euclidean metric on $\mathbb{C} = \mathbb{R}^2$, [31]. If one adopts the arc-length parametrization $\gamma(x)$ of Γ , the contribution to the induced integral measure is identically 1, and the L^2 -inner product along Γ has the form

$$\langle \Psi | \Phi \rangle_\Gamma := \int_\Gamma \Psi(z)^* \Phi(z) dz = \int_{\mathbb{R}} \Psi(\gamma(x))^* \Phi(\gamma(x)) dx. \quad (6)$$

The above discussion suggests that the state space \mathcal{V}_Γ is to be identified as a (topological) vector space with the Hilbert space

$$L^2(\Gamma) := \{\Psi : \Gamma \rightarrow \mathbb{C} \mid \langle \Psi | \Psi \rangle_\Gamma < \infty\}.$$

This is a consequence of purely mathematical considerations. The state space \mathcal{V}_Γ is furthermore required to be a separable Hilbert space with an inner product that renders

the Hamiltonian operator H self-adjoint. As we show in the remainder of this section this is a direct and unavoidable consequence of the measurement axiom which we intend to adopt. Specifically, we assume the following.

- (i) There is a positive-definite inner product $\langle \cdot, \cdot \rangle_+ : \mathcal{V}_\Gamma^2 \rightarrow \mathbb{C}$ on \mathcal{V}_Γ such that $\mathcal{H}_{\text{phys}} := (\mathcal{V}_\Gamma, \langle \cdot, \cdot \rangle_+)$ is a separable Hilbert space.
- (ii) The (pure) states of the system are in one-to-one correspondence with the rays (one-dimensional subspaces) of $\mathcal{H}_{\text{phys}}$ each of which is described by a nonzero state vector $\Psi \in \mathcal{H}_{\text{phys}}$.
- (iii) The observables O of the theory are linear operators acting in $\mathcal{H}_{\text{phys}}$.
- (iv) Suppose that O is an observable having a discrete spectrum³ and that the system is in the state described by the state vector Ψ . Upon measuring O , the state of the system collapses onto a state described by a state vector Ω_n . The measuring device records ω_n if and only if Ω_n is an eigenvector of O with eigenvalue ω_n . The probability of measuring ω_n is given by

$$\text{Prob}_n(\Psi) := \frac{\langle \Lambda_n \Psi, \Lambda_n \Psi \rangle_+}{\langle \Psi, \Psi \rangle_+}, \quad (7)$$

where Λ_n is the projection operator⁴ onto the subspace of \mathcal{V}_Γ consisting of the eigenvectors of O with eigenvalue ω_n .

- (v) The probability $\text{Prob}_n(\Psi)$ of measuring ω_n is a continuous function of time, i.e., if one measures ω_n at time $t = 0$ and repeats the same measurement at time $t > 0$, the probability of measuring a different eigenvalue than ω_n tends to zero as $t \rightarrow 0$.

Because measuring devices read real numbers, the spectrum of an observable is necessarily real. Furthermore, the following two physical requirements imply that the set $\text{Span}(O)$ of linear combinations of the eigenvectors of O must be dense in $\mathcal{H}_{\text{phys}}$.

- (a) There is a dense set \mathcal{D} of elements Ψ of $\mathcal{H}_{\text{phys}}$ that describe states of the system in which O can be measured⁵;
- (b) The probability of all possible outcomes of a measurement must add up to unity.

Note also that (iv) puts a strong restriction on the projection operators, namely that $\Lambda_m \Lambda_n = \delta_{mn} \Lambda_n$. This implies the existence of an orthogonal basis of $\mathcal{H}_{\text{phys}}$ consisting

³The case of continuum spectrum can be treated similarly [26].

⁴It is a linear operator acting in \mathcal{V}_Γ and satisfying $\Lambda_n^2 = \Lambda_n$.

⁵This means that every nonzero state vector $\Psi \in \mathcal{H}_{\text{phys}}$ describes a physically accessible state of the system; it can be approximated with any desired accuracy by the elements of \mathcal{D} .

of the eigenvectors of O .⁶ This together with the reality of the spectrum of O yield the condition: “ O must be a densely defined self-adjoint operator acting in $\mathcal{H}_{\text{Phys}}$.”

It should be emphasized that *although the measurement axiom does not fix or restrict the choice of the defining inner product of the physical Hilbert space, it makes the self-adjointness of the observables absolutely necessary.* The condition of the Hermiticity of the observables O and in particular the Hamiltonian that is adopted in the conventional quantum mechanics is therefore a valid and indisputable condition provided that it is interpreted as self-adjointness of O as an operator acting in the physical Hilbert space $\mathcal{H}_{\text{Phys}}$, i.e., for every Ψ and Φ in the domain of O ,

$$\langle \Psi, O\Phi \rangle_+ = \langle O\Psi, \Phi \rangle_+. \quad (8)$$

This may be called *Hermiticity with respect to the inner product $\langle \cdot, \cdot \rangle_+$* . This is not the same notion of *Hermiticity* that is used in the literature in \mathcal{PT} -symmetry. The latter is defined in terms of a pre-assigned *reference inner product $\langle \cdot | \cdot \rangle$* that is generically different from $\langle \cdot, \cdot \rangle_+$ and hence physically inadmissible. The typical example of the reference inner product $\langle \cdot | \cdot \rangle$ is the L^2 -inner product $\langle \cdot | \cdot \rangle_{\Gamma}$ of Eq. (6). Therefore the answer to the question posed in the title of this section and that of [33] is that it depends on the definition of the term “Hermitian.” If one defines it with respect to the L^2 -inner product which is equivalent to saying that O is Hermitian if it can be expressed as the integral operator,

$$(O\Psi)(\gamma(x)) = \int_{\mathbb{R}} O(x, y) \Psi(\gamma(y)) dy,$$

with a kernel satisfying $O(x, y)^* = O(y, x)$ for all $x, y \in \mathbb{R}$, then the answer is NO. But this answer must be qualified by saying that O must nevertheless be Hermitian with respect to some positive-definite inner product $\langle \cdot, \cdot \rangle_+$. The issue of the existence and construction of $\langle \cdot, \cdot \rangle_+$ is currently a subject of active research [9, 16, 34, 14, 35, 15, 36, 37, 38, 39]. For an earlier investigation see [40].

3 The Krein-Space or Indefinite-Metric Formulation

Let \mathcal{V} be a complex vector space. Then a function $Q : \mathcal{V}^2 \rightarrow \mathbb{C}$ with domain \mathcal{V}^2 is said to be a [41]

- *nondegenerate form*, if “for all $v \in \mathcal{V}$, $Q(v, w) = 0$ ” implies “ $w = 0$ ”;
- *Hermitian form*, if $Q(v, w)^* = Q(w, v)$ for all $v, w \in \mathcal{V}$;
- *sesquilinear form*, if $Q(u, \alpha v + \beta w) = \alpha Q(u, v) + \beta Q(u, w)$ and $Q(\alpha u + \beta v, w) = \alpha^* Q(u, w) + \beta^* Q(v, w)$, for all $u, v, w \in \mathcal{V}$ and $\alpha, \beta \in \mathbb{C}$;

⁶The generalization of the situation for the cases that the spectrum of O is not discrete leads to the requirement that O has a spectral resolution of the identity [32].

- *positive-definite form*, if $Q(v, v) \in \mathbb{R}^+$ for all $v \in \mathcal{V} - \{0\}$.

Furthermore, if \mathcal{V} is endowed with a norm [41] denoted by $\|\cdot\|$, then Q is called a

- *bounded form*, if there exists $c \in \mathbb{R}^+$ such that $|Q(v, w)| \leq c \|v\| \|w\|$ for all $v, w \in \mathcal{V}$.

A non-degenerate Hermitian sesquilinear form is called a *pseudo-inner product*. A positive-definite pseudo-inner product is called a *positive-definite inner product* or simply an *inner product*. A pseudo-inner product that is not positive-definite is called an *indefinite inner product*.

If one endows \mathcal{V} both with a norm $\|\cdot\|$ and a bounded positive-definite inner product $\langle \cdot, \cdot \rangle := Q(\cdot, \cdot)$, then the norm $\sqrt{\langle \cdot, \cdot \rangle}$ associated with $\langle \cdot, \cdot \rangle$ defines a topology on \mathcal{V} which is identical with the topology defined by the defining norm $\|\cdot\|$.⁷

Suppose that $\langle \cdot, \cdot \rangle$ is a positive-definite inner product on \mathcal{V} and $\|\cdot\| := \sqrt{\langle \cdot, \cdot \rangle}$ is the corresponding norm. It is not difficult to show that there is a one-to-one correspondence, given by

$$Q_T(v, w) = \langle v, Tw \rangle, \quad (9)$$

between bounded sesquilinear forms Q_T on \mathcal{V} and everywhere-defined bounded linear operators $T : \mathcal{V} \rightarrow \mathcal{V}$, [41]. If Q_T is non-degenerate (respectively, Hermitian or positive-definite), T is invertible (respectively, self-adjoint or positive-definite). Here invertible means that T is one-to-one, onto, and T^{-1} is bounded [41], self-adjoint means: $\langle v, Tw \rangle = \langle Tv, w \rangle$ for all $v, w \in \mathcal{V}$, and positive-definite means: $\langle v, Tv \rangle \in \mathbb{R}^+$ for all $v \in \mathcal{V} - \{0\}$.

A *Krein Space* [7] is a complex vector space \mathcal{V} that is endowed with an indefinite inner product (\cdot, \cdot) and has a pair of vector subspaces \mathcal{V}_\pm with the following properties.

- $\pm(v_\pm, v_\pm) > 0$ for all $v_\pm \in \mathcal{V}_\pm - \{0\}$;
- \mathcal{V}_- and \mathcal{V}_+ are orthogonal, i.e., $(v_+, v_-) = 0$ for all $v_\pm \in \mathcal{V}_\pm - \{0\}$;
- \mathcal{V} is a direct sum of \mathcal{V}_- and \mathcal{V}_+ ,

$$\mathcal{V} = \mathcal{V}_- \oplus \mathcal{V}_+, \quad (10)$$

i.e., for all $v \in \mathcal{V}$ there are unique $v_\pm \in \mathcal{V}_\pm$ such that $v = v_- + v_+$;

- \mathcal{V}_\pm endowed with the positive-definite inner products obtained by restricting $\pm(\cdot, \cdot)$ onto \mathcal{V}_\pm are separable Hilbert spaces.

A principal result of the theory of Krein spaces is that a Krein space may be endowed with a positive-definite inner product $\langle \cdot, \cdot \rangle_+ : \mathcal{V}^2 \rightarrow \mathbb{C}$ and turned into a separable Hilbert

⁷This means that both norms define the same notion of the convergence for sequences in \mathcal{V} .

space. This is achieved using the projection operators $\Pi_{\pm} : \mathcal{V} \rightarrow \mathcal{V}$ associated with the orthogonal direct sum decomposition (10); Π_{\pm} projects every $v \in \mathcal{V}$ onto its component v_{\pm} in \mathcal{V}_{\pm} . Clearly, $\Pi_{-} = I - \Pi_{+}$, where I denotes the identity operator acting in \mathcal{V} . The inner product $\langle \cdot, \cdot \rangle_{+}$ has the form [19, 7, 3, 42]:

$$\langle v, w \rangle_{+} := (\Pi_{+}v, \Pi_{+}w) - (\Pi_{-}v, \Pi_{-}w) = (v, Cw), \quad (11)$$

where

$$C := \Pi_{+} - \Pi_{-} = 2\Pi_{+} - I. \quad (12)$$

The operator C is actually a *grading operator*, for

$$\mathcal{V}_{\pm} = \{v \in \mathcal{V} \mid Cv = \pm v\}. \quad (13)$$

In particular it is an involution: $C^2 = I$. This operator which in the mathematical literature is usually denoted by J and referred to as the “*fundamental symmetry operator*” [42] is precisely the “charge-conjugation operator” of Bender, Brody, and Jones [16] whenever the Krein-space theory is applied in the study of \mathcal{PT} -symmetric Hamiltonians [20, 21].

Because \mathcal{V} endowed with $\langle \cdot, \cdot \rangle_{+}$ is a separable Hilbert space that admits the direct sum decomposition (10), there is an orthonormal basis $\{\xi_n^{\pm}\}$ of this Hilbert space such that $\xi_n^{\pm} \in \mathcal{V}_{\pm}$ for all $n = 0, 1, 2, \dots$. We can relabel the basis vectors according to

$$\xi_n^{\pm} \rightarrow \psi_n := \begin{cases} \xi_{\frac{n}{2}}^{+} & \text{for } n \text{ is even} \\ \xi_{\frac{n-1}{2}}^{-} & \text{for } n \text{ is odd.} \end{cases} \quad (14)$$

This yields

$$\langle \psi_m, \psi_n \rangle_{+} = \delta_{mn}, \quad m, n = 0, 1, 2, \dots, \quad (15)$$

and, in view of (11) and (13) – (15),

$$(\psi_m, \psi_n) = (-1)^m \delta_{mn}, \quad m, n = 0, 1, 2, \dots. \quad (16)$$

Furthermore, we have

$$C = \sum_n (-1)^n \Lambda_n, \quad (17)$$

where Λ_n denotes the projection operator defined by

$$\Lambda_n w := \langle \psi_n, w \rangle_{+} \psi_n, \quad \text{for all } w \in \mathcal{V}. \quad (18)$$

Next, consider the case that \mathcal{V} has the structure of a separable Hilbert space with another inner product $\langle \cdot | \cdot \rangle : \mathcal{V}^2 \rightarrow \mathbb{C}$ such that the corresponding norm $\| \cdot \|$ defines the same topology as the norm $\| \cdot \|_{+}$ associated with the inner product $\langle \cdot, \cdot \rangle_{+}$. Let us denote the Hilbert space $(\mathcal{V}, \langle \cdot | \cdot \rangle)$ by \mathcal{H} and the Hilbert space $(\mathcal{V}, \langle \cdot, \cdot \rangle_{+})$ by \mathcal{H}_{+} . Then, as we

mentioned above, there is an everywhere-defined, bounded, positive-definite, invertible operator $\eta_+ : \mathcal{H} \rightarrow \mathcal{H}$ such that [41]

$$\langle \cdot, \cdot \rangle_+ = \langle \cdot | \eta_+ \cdot \rangle. \quad (19)$$

Similarly we have an everywhere-defined, bounded, self-adjoint, invertible operator $P : \mathcal{H} \rightarrow \mathcal{H}$ such that⁸

$$(\cdot, \cdot) = \langle \cdot | P \cdot \rangle. \quad (20)$$

Combining (11), (19), and (20), we have [18, 13]

$$C = C^{-1} = \eta_+^{-1} P. \quad (21)$$

Because the span of the vectors ψ_n is a dense subset of \mathcal{H} , we can identify $\{\psi_n\}$ with a basis of \mathcal{H} . It is important to note that in general this basis fails to be orthogonal.

Next, observe that the unique positive square root $\rho = \sqrt{\eta_+}$ of η_+ viewed as an operator mapping \mathcal{H}_+ onto \mathcal{H} satisfies

$$\langle \rho v | \rho w \rangle = \langle v | \eta_+ w \rangle = \langle v, w \rangle_+, \quad \text{for all } v, w \in \mathcal{H}_+. \quad (22)$$

Hence $\rho : \mathcal{H}_+ \rightarrow \mathcal{H}$ is a unitary operator [44]. A simple consequence of (22) is that $\zeta_n := \rho \psi_n$ form an orthonormal basis of \mathcal{H} . Because η_+ is an everywhere-defined bounded invertible operator, so is its square root ρ . This in turn means that $\{\psi_n\}$ is related to an orthonormal basis $(\{\zeta_n\})$ via a bounded invertible operator. Such a basis is called a *Riesz basis*, [45]. A characteristic property of every Riesz basis is that it can be extended to a biorthonormal system [45], i.e., there is a (Riesz) basis $\{\phi_n\}$ of \mathcal{H} , such that

$$\langle \phi_m | \psi_n \rangle = \delta_{mn}, \quad (23)$$

$$\sum_n \langle \phi_n | w \rangle \psi_n = \sum_n \langle \psi_n | w \rangle \phi_n = w \quad \text{for all } w \in \mathcal{H}. \quad (24)$$

Rewriting the latter relation using the Dirac notation one finds the familiar condition [8, 9]:

$$\sum_n |\psi_n\rangle \langle \phi_n| = I = \sum_n |\phi_n\rangle \langle \psi_n|. \quad (25)$$

In view of (15), (19), and (23), we can relate ϕ_n to ψ_n via

$$\phi_n = \eta_+ \psi_n. \quad (26)$$

Inserting this equation in (18) and using (19) and the self-adjointness of η_+ , we then find

$$\Lambda_n \psi = \langle \psi_n | \psi \rangle_+ \psi_n = \langle \psi_n | \eta_+ \psi \rangle \psi_n = \langle \eta_+ \psi_n | \psi \rangle \psi_n = \langle \phi_n | \psi \rangle \psi_n, \quad \text{for all } \psi \in \mathcal{H}.$$

⁸As I explain in [43], an everywhere-defined self-adjoint operator is necessarily bounded and the onto-ness of P ensures that its inverse is bounded. Hence the conditions listed here may be summarized as: “ P is a Hermitian (self-adjoint) automorphism,” [8].

We can express this result using the Dirac notation in the form:

$$\Lambda = |\psi_n\rangle\langle\phi_n|. \quad (27)$$

Combining this relation with (17), we have

$$C = \sum_n (-1)^n |\psi_n\rangle\langle\phi_n|. \quad (28)$$

This equation was initially derived in [18] in an attempt to show how the results of [16] relate to those of [9].

Next, we use (26), (25), (21), and (28) to establish

$$\eta_+ = \sum_n |\phi_n\rangle\langle\phi_n|, \quad (29)$$

$$\eta_+^{-1} = \sum_n |\psi_n\rangle\langle\psi_n|, \quad (30)$$

$$P = \sum_n (-1)^n |\phi_n\rangle\langle\phi_n|. \quad (31)$$

These are among the basic equations of the pseudo-Hermitian treatment of \mathcal{PT} -symmetric Hamiltonians developed in [8, 9, 17, 18]. It is absolutely essential to realize that the analysis leading to (28) – (31) applies in any Krein-space setting.

4 Boundedness of the Metric and Diagonalizability of the Hamiltonian

In applying the properties of pseudo-Hermitian operators [8] to \mathcal{PT} -symmetric Hamiltonians H that have a real and discrete spectrum, one adopts a separable (reference) Hilbert space \mathcal{H} containing the domain of H as a dense subset (so that the adjoint H^\dagger of H is well-defined [46]) and assumes that as an operator acting in \mathcal{H} the Hamiltonian H is diagonalizable [9, 17, 12]. This precisely means that there is a Riesz basis $\{\psi_n\}$ of \mathcal{H} consisting of the eigenvectors of H .⁹ The fact that as a vector space the Hilbert space must only include the closed span of the eigenvectors of H is a physical necessity.¹⁰ Therefore, the existence of a basis consisting of the eigenvectors of H is easy to justify. The additional condition that this basis be a Riesz basis is a mathematical requirement. One can enforce it by choosing an appropriate reference Hilbert space \mathcal{H} , i.e., an appropriate inner product $\langle\cdot|\cdot\rangle$ on the vector space of state vectors that renders the latter a separable Hilbert space. The condition that such an inner product must exist is a physical requirement on H . But the choice of $\langle\cdot|\cdot\rangle$ is not dictated by physics and can be made arbitrarily. For example one

⁹A direct consequence of the identification of ψ_n with the eigenvectors of H is $[C, H] = 0$.

¹⁰Otherwise, there will be states for which H cannot be measured!

may define the Hilbert space of the theory by taking the span of the eigenvectors of H , endow it with the inner product that renders the eigenvectors orthonormal, and complete the resulting inner product space into a Hilbert space as proposed by Kretschmer and Szymanowski [49].

The approach of [49] directly gives the physical Hilbert space of the system, but in essence uses a representation of the system that is based on the Hilbert space ℓ_2 of square summable complex sequences [50]. In this representation the Hamiltonian enters only in the form of its eigenvalues. Furthermore, in view of the form of the inner product on ℓ_2 :

$$\langle \{s_n\}, \{t_n\} \rangle := \sum_{n=0}^{\infty} s_n^* t_n,$$

the calculation of physical quantities, such as the expectation value of observables, involves summing complicated series. To avoid dealing with such an important practical problem, one maps ℓ_2 onto L_2 by an appropriate unitary operator and performs the calculations in this representation that uses L_2 as the physical Hilbert space of the system. Alternatively, one may perform a unitary mapping of the physical Hilbert space onto L_2 directly to arrive at this L^2 -representation [49]. The fact that this can always be done is a well-known consequence of the uniqueness theorem for infinite-dimensional separable Hilbert spaces [50]. But there is no unique or systematic (canonical) way of choosing this unitary mapping and the corresponding alternative L^2 -representation. One is naturally inclined to determine and make a choice in which the Hamiltonian takes a simpler form in the L^2 -representation. How one can achieve this, however, is not known to the present author.

The main advantage of the method of [49] is that it avoids the technical problems related to the boundedness of the metric operators. As we mentioned above the metric operators η_+ that define (topologically equivalent) positive-definite inner products are necessarily everywhere-defined, bounded, and invertible. These conditions are sometimes ignored in constructing concrete examples of a metric operator for models typically defined in $\mathcal{H} = L^2(\Gamma)$. These constructions involve obtaining an operator η_+ that satisfies the pseudo-Hermiticity condition

$$H^\dagger = \eta_+ H \eta_+^{-1}, \tag{32}$$

is formally Hermitian, i.e., there is a dense subset $\mathcal{S} \subseteq \mathcal{H}$ in which $\eta_+^\dagger = \eta_+$, and positive-definite, i.e., η_+ has a real positive-definite spectrum. Such an operator defines an inner product on \mathcal{S} . The resulting inner product is generally incomplete. It can be completed to a separable Hilbert space. But the resulting space generally differs from \mathcal{H} , for they have different topologies.¹¹ This observation is sometimes viewed as a shortcoming of the pseudo-Hermitian treatment of \mathcal{PT} -symmetric systems [49]. This view seems to ignore

¹¹Such non-invertible or unbounded “metric operators” have an important application [51] in the context of the method of complex scaling in the study of resonances [52].

the fact that the failure to construct examples of metric operators that satisfy all the above-mentioned conditions cannot be accepted as a proof of their nonexistence.

The pseudo-Hermitian treatment of the \mathcal{PT} -symmetric models considered in [8, 9, 13] is based on choosing $L^2(\Gamma)$ as the reference Hilbert space \mathcal{H} . This has the advantage of making the relationship between the usual Hermitian quantum mechanics, where \mathcal{H} is the physical Hilbert space, more transparent. Indeed, this approach is the only known one that allows for the determination of an underlying classical system (with the correct number of degrees of freedom [53]) and a consistent quantization scheme that links the latter to the original quantum system, [12, 14, 15]. These are absolutely essential for assigning physical meaning to the operators that one identifies with the observables of the theory. The only disadvantage of this approach is the possibility that H may turn out to be non-diagonalizable as an operator acting in $L^2(\Gamma)$, i.e., there exists a set of Hilbert spaces \mathcal{H} in which H acts as a diagonalizable operator but $L^2(\Gamma)$ does not belong to this set.

Contrary to the claims made in [23], the requirement of the existence of a biorthonormal system consisting of eigenvectors of the Hamiltonian operator and its adjoint is well-justified by physical considerations. According to quantum measurement theory, one cannot call a (differential) operator H “the Hamiltonian of a unitary quantum system,” if the set of its eigenvectors is incomplete or more generally if there does not exist a separable Hilbert space in which H acts as a densely defined self-adjoint operator.¹²

In practice, given a differential operator H with a well-posed eigenvalue problem, one has access to its domain as a function space. To embed this space (as a closed subspace) in a reference Hilbert space \mathcal{H} such that the set of eigenvectors of H form a Riesz basis of \mathcal{H} is a mathematical problem that must be considered separately from the eigenvalue problem for H . If such a Hilbert space does not exist, H is not a viable candidate for the Hamiltonian operator of a physical system. If such a Hilbert space exists then the eigenvectors of H form a Riesz basis and they can be extended to a biorthonormal system, i.e., as an operator acting in \mathcal{H} , H is diagonalizable. Determining the class of differential operators fulfilling this condition is an interesting and admittedly difficult mathematical problem.

The physical problem may be devised and investigated only after one is provided with a differential operator H and a separable Hilbert space \mathcal{H} in which H is diagonalizable. Clearly there are an infinity of (unitarily equivalent) separable Hilbert spaces \mathcal{H} rendering such a differentiable operator diagonalizable. All these choices are clearly physically equivalent [50] and for all of them the construction outlined in [9] for a physically admissible positive-definite inner product applies. The question whether $L^2(\Gamma)$ is among the possible choices for \mathcal{H} must be addressed for each H separately. Based on numerical

¹²A class of examples of such operators are those involving spectral singularities [47, 48].

evidence it is assumed that this is the case for most \mathcal{PT} -symmetric potentials considered in the literature [16].

5 Concluding Remarks

The postulate that physical states of a quantum system are represented by rays in a separable Hilbert space and the quantum measurement postulate are as indispensable for any quantum theory, as is the Schrödinger time evolution. This is independent of whether one begins with a mathematical formalism that does not involve a Hilbert space structure from the outset. A serious attempt to formulate a genuine generalization of (or an alternative to) quantum mechanics must begin with a clear and comprehensive description of its postulates. This must follow with a discussion of interpretational issues. A mathematical scheme for achieving such a theory, however rigorous it may be, is to be rejected, if it does not obey the conditions set by the physical reality. The history of modern physics shows that the main guidelines for real progress are physical considerations.

Imposition of the demands of physics upon mathematical models is also a delicate issue. One must be extremely careful in ascribing the property of being *physical* to a mathematical construct. For example, some of the workers on the subject use the following argument as a motivation for their investigations: “ \mathcal{PT} -symmetry is a more physical condition than Hermiticity, because it means space-time reflection symmetry.” This would be true, if the parity operator \mathcal{P} described “space-reflection.” This happens if and only if the space, i.e., the position observable of a particle, is identified with the usual x operator. The latter is well-known not to be an observable in almost all known \mathcal{PT} -symmetric models. For these models, therefore, \mathcal{PT} does not describe a space-time reflection, and *\mathcal{PT} -symmetry is not a physical symmetry* as claimed. This overshadows the physical viability of formulations that take the operator \mathcal{P} or \mathcal{PT} as the fundamental building block [22, 23] as opposed to the Hilbert space structure [12, 50].

In general, in order for \mathcal{P} to describe a space-reflection, the model(s) under consideration must admit the x operator as an observable and there must exist a correspondence principle that relates this operator to the classical position of a particle. Before specifying an underlying classical system and formulating a quantization scheme that maps the classical observables to their quantum analogs, one cannot assign any physical meaning to the latter. This is the fundamental reason why one needs a *correspondence principle* in any quantum theory.

The surprising spectral properties of \mathcal{PT} -symmetric potentials have initially made the impression that these potentials may be a basis for an extension of quantum mechanics [16]. This turned out not to be true in the sense that such a theory, even if it is formulated in a consistent manner, will be equivalent to the conventional quantum mechanics [55, 50].

What is true is that the formulation based on \mathcal{PT} -symmetric or more generally pseudo-Hermitian Hamiltonians yields an alternative (pseudo-Hermitian) representation of the conventional quantum mechanics. The availability of this representation seems to have been overlooked for over seventy years. Its recent discovery [44, 12] seems to offer a new prospective for dealing with a number of important problems of mathematical/theoretical physics.

A concrete example of the application of the pseudo-Hermitian representation of quantum mechanics is the solution of the Hilbert-space problem for Klein-Gordon fields in relativistic quantum mechanics and Wheeler-DeWitt fields in minisuperspace quantum cosmology [11]. Another more recent example is the treatment of position-dependent-mass Hamiltonians reported in [54]. It is based on the observation that some complex \mathcal{PT} -symmetric potentials define systems that are perturbatively equivalent to those described by a standard Hermitian Hamiltonian with a position-dependent mass [14].

The fact that systems defined by \mathcal{PT} -symmetric potentials admit a Hermitian description [44] is not only instrumental in determining the observables and the classical limit of these systems [12], but it plays an important role in understanding the spectral properties of the wrong-sign quartic potential [56]. Another, perhaps more important, application of the equivalence of the Hermitian and pseudo-Hermitian representations of quantum mechanics is a novel resolution of the old and practically important problem of bound state scattering [57].

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